Institute for Materieals Science Lecture Series

'D'++: Going Beyond DFT via GW and Vertex Corrections

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Date: Wednesday, February 17, 2016
Time: 2:00 – 3:00pm
Location: MSL Auditorium (TA-03 - Bldg 1698 - Room A103)

Abstract: A large variety of approaches have been implemented for extending DFT (density-functional theory) calculations of band structure to account for stronger calculations. In particular, GW calculations are used to calculate the electronic self-energy, but there is debate about whether non-self-consistent [or G0W0] or self-consistent [GW] calculations perform better. We have found that as correlation strength increases the G0W0 approach fails, but that this can be corrected by a self-consistent approach, called quasiparticle-GW [QPGW] or GZWZ. While considerably simpler than full GW, this new approach has proven to be readily adaptable to a variety of spectroscopies, giving good agreement for a number of properties of cuprates. In particular, the high momentum-space resolution has allowed the observation of competing density-wave phases in the phase diagrams of many cuprates.

While the QPGW approach provides a good starting point for most spectroscopies, the finite-temperature results are limited in that the phase transitions are mean-field. Thus, the superconducting transition lies at too high a temperature when short-range fluctuations are important. Worse, the pseudogap is classified as merely a mean field antiferromagnetic transition. To better understand pseudogap physics, we have recently extended the GW calculation to include a self-consistent vertex correction. This reveals that pseudogap physics is a strong coupling effect: significant mode-coupling leads to a breakdown of the random-phase approximation and a condensation bottleneck, leading to extended ranges of short-range order.
(Tanmoy Das, R. S. Markiewicz, A. Bansil, Advances in Physics 63, 151-266 (2014) / R.S. Markiewicz, I.G. Buda, P. Mistark, A. Bansil, arXiv:1505.04770)

Bio: Bob Markiewicz got his Ph.D. in Berkeley in 1976, studying electron-hole droplets in Ge [Kittel, ISSP, 8th. Ed., Fig. 15.12]. After a two-year Post-Doc, he joined the Research Staff at G.E. in Schenectady, N.Y., where he studied graphite intercalation compounds and localization in ultrathin metal films. In 1980 he moved to Northeastern University in Boston, where he began studying cuprate physics in 1987, concentrating mainly on nanoscale phase separation and the role of the Van Hove singularity.

Around 2000 he began an ongoing collaboration with Arun Bansil at NU, to extend first-principles density-functional theories to study spectroscopies and more strongly-correlated materials. They initially studied ARPES [angle-resolved photoemission spectroscopy], and found that electron-doped cuprates were much simpler to understand, involving only (pi,pi) antiferromagnetism and superconductivity. He developed a form of DFT+GW calculation which could be applied to a variety of spectroscopies, including STM, optical, neutron scattering, and RIXS, and analyzed the competing-order phase diagrams of hole-doped cuprates, finding that LSCO is significantly different from other cuprates. He is now extending these calculations to include vertex corrections necessary to understand pseudogap physics.

He has also worked on SO(8), stripe physics, Fermi surface nesting, edge singularities in RIXS, and negative compressibility.

Hosted By Alexander Balatsky